APPENDIX I

DESCRIPTION OF COMPUTER MODELING PROCEDURES FOR METHYL BROMIDE

State of California

Memorandum

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From: **Department of Pesticide Regulation** - 1020 N Street, Room 161
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Subject: DESCRIPTION OF COMPUTER MODELING PROCEDURES FOR METHYL BROMIDE

Background

Methyl bromide is a colorless (a dye is sometimes added) and odorless (a warning agent is usually added) gas at normal pressure and temperature. It is one of the most widely used pesticides, with 15 - 20 million pounds applied annually in California over the last few years. It is registered as a soil fumigant, as a fumigant for food and nonfood commodities, and for pest control in buildings. The largest quantity of methyl bromide is used as a soil fumigant prior to planting in agricultural fields.

Methyl bromide manufacturers test the toxicity of methyl bromide using animals. The most recent test results evaluated by Department of Pesticide Regulation (DPR) scientists indicate toxic effects at doses lower than previously documented (Nelson 1992). Based on the animal test data, DPR estimates that the level that causes no observable effects in people is 21 parts per million of methyl bromide in air. To ensure an adequate margin of safety, DPR adds a 100-fold safety factor and uses a target level of 0.21 parts per million (24-hour average concentration) for its regulatory program.

Numerous monitoring studies have documented air concentrations of methyl bromide near fumigation areas during and after methyl bromide applications (Ross, et al. 1996; Siemer and Hicks 1993). In several instances, measured air concentrations exceeded DPR's target level. DPR and county agricultural commissioners have implemented several restrictions or conditions on methyl bromide applications to ensure people's exposure does not exceed DPR's target level. These conditions include buffer zones that must be maintained between the application area and places where people conduct certain activities. DPR uses field monitoring data in conjunction with computer modeling to determine the appropriate buffer zone sizes.

Description of Computer Model

One of the major drawbacks to field monitoring is that it can only determine air concentrations at specific locations at specific times. Extrapolating these data to other locations and times is usually very difficult. To overcome this drawback, DPR uses methyl bromide monitoring data in conjunction with a computer model, the Industrial Source Complex-Short Term (ISCST) model. The U.S. Environmental Protection Agency developed this model for air pollution simulation, but it has rarely been applied to agricultural situations. The current buffer zones for methyl bromide are based on the first version of the ISCST model published in 1987. The most recent update, version 3 of the model, was published in 1995. Version 3 is the first update in which the basic equations for simulating air concentrations have been modified. DPR is reanalyzing the monitoring data and revising the buffer zones based on version 3 of the model.

The ISCST model assumes that all movement of a pollutant is due to air currents; wherever the wind blows that is where the methyl bromide will go. The ISCST model simulates air concentrations based on three main factors: (1) characteristics of the pollution source, such as rate of emission and size of the field; (2) weather conditions at the time of emission, such as wind speed and wind direction; and (3) terrain over the downwind area, such as urban or rural geography. These three factors are discussed in detail below. A pictorial representation of the model is shown in Figure 1.

Source Characteristics Used by the ISCST Model

For agricultural fields, the methyl bromide source is characterized primarily by two parameters: the emission or flux rate and the size of the field. The flux rate is the amount of methyl bromide released to the air from a given area and in a given time period; for example, 100 pounds of methyl bromide per acre per day. All other factors being equal, the greater the flux rate, the higher the air concentrations. In fact, the ISCST model assumes that the flux rate and air concentration are directly proportional; if the flux rate doubles, the air concentration doubles. Similarly, the larger the area, the higher the air concentrations. However, this relationship is not directly proportional; if the area doubles, the air concentration less than doubles.

Numerous physical and chemical characteristics influence the methyl bromide flux rate. Probably the primary factor in determining the flux rate is the application rate. The higher the application rate, the higher the flux rate. Other factors that affect the flux rate include the method of application, soil characteristics, and temperature. The ISCST model does not directly simulate these factors; and their effect on the flux rate must be determined from experimental data.

Weather Data Used by the ISCST Model

Wind speed effects air concentrations. The higher the wind speed, the lower the air concentration. Wind direction is the primary factor that determines the location of methyl bromide in air. The ISCST model assumes that methyl bromide will move as a plume or cloud in the downwind direction. Wind direction, or more precisely, the variation in wind direction also influences air concentrations. When the wind direction is constant, the plume is narrow and the air concentrations of methyl bromide are relatively higher. When the wind direction is variable, the plume is wide and the air concentrations of methyl bromide are relatively lower.

Atmospheric stability also has a major influence on air concentrations. Atmospheric stability refers to vertical mixing of the air due to heating or convection and is classified from A to F—with A the least stable and F the most stable (Pasquill 1961). In general, the more stable the atmosphere, the higher the air concentrations. Normally, there is daily variation in atmospheric stability. The air becomes well-mixed (A-most unstable) during the day as the ground heats up. The air does not mix (F-most stable) during the night as the ground cools. Atmospheric stability also varies seasonally. The atmosphere is more stable during the winter due to longer nights in comparison to summer which has shorter nights.

Terrain Data Used by the ISCST Model

The type of terrain also influences air concentrations because terrain influences atmospheric stability. All other factors being equal, rural areas have more stable air and thus higher air concentrations of methyl bromide than urban areas. Urban areas have less stable air due to numerous heat sources (e.g., asphalt) and obstructions (e.g., buildings) and thus have relatively lower air concentrations of methyl bromide.

Unaccounted Factors/Model Shortcomings

Measured methyl bromide air concentrations generally show good agreement with those simulated by the ISCST model. However, there are some situations that the ISCST model does not simulate well, either due to shortcomings of the input data for the model or because the model does not account for all processes or circumstances. For example, the ISCST model does not simulate long periods of low or zero wind speed. It is also difficult to account for low inversion layers. A low inversion layer is an area of the atmosphere that has a higher temperature than the air below it and acts as a cap, causing higher air concentrations of methyl bromide close to the ground. While the height of an inversion layer can be input into the model, this parameter is difficult to determine in the field and generally a default value of 700 meters is used.

Method for Evaluating Monitoring Data Using the ISCST Model

As discussed above, the ISCST model uses the flux rate, field size, weather, and terrain to simulate air concentrations. In the case of methyl bromide, field studies provide data on the field size, weather, terrain, and air concentrations, but not the flux rate. Determining the flux rate requires special equipment unavailable during previous studies. In order to use the ISCST model to simulate air concentrations under a variety of weather and terrain conditions, DPR uses the ISCST model to "back-calculate" an estimate of methyl bromide flux rates.

DPR back-calculates flux rates using a two-step process (Ross 1996). First, the known field size, weather, and terrain data from a field study are input into the ISCST model. An assumed flux rate is also input into the ISCST model. Second, the air concentrations simulated by the ISCST model (using the assumed flux value) are then statistically compared to the measured air concentrations. The comparison of measured and simulated air concentrations yields an adjustment or calibration factor for the assumed flux value. Using the calibrated flux value in the ISCST model gives the best match to the measured air concentrations. This flux calibration factor represents the flux rate for modeling purposes.

The flux calibration provides an estimate of the flux rate plus any other factors. As discussed previously, the ISCST model does not account for all factors that may influence methyl bromide air concentrations. If the unaccounted factors have little influence on air concentrations, then the flux calibration factor is close to the actual flux rate. But if the unaccounted factors play a major role in air concentrations, then the flux calibration factor accounts for the flux rate plus the other factors. The strength of this procedure allows the model to account for factors difficult to measure. For example, DPR assumes that any inversion layer is high and has little effect on air concentrations. However, if one of the field studies had higher air concentrations caused by a low inversion layer, then the back-calculation procedure results in a higher flux calibration factor in order to account for the higher air concentrations. In other words, DPR's modeling procedure accounts for low inversions by increasing the flux rate. A pictorial representation of the back-calculation procedure is shown in Figure 2. The flux calibration factor resulting from the back-calculation is one of the main variables that determines the size of the buffer zone.

Determination of Buffer Zone Sizes

Five main parameters determine the size of the buffer zones: the flux calibration factor, the number of acres treated, assumed weather conditions, assumed terrain, and the target air concentration.

Flux Calibration Factor

DPR assumes that the flux rate (or flux calibration factor) of methyl bromide is directly proportional to the application rate; if the application rate doubles, the flux rate doubles (the ISCST model assumes the flux rate and air concentrations are directly proportional). Therefore, DPR adjusts the flux calibration factor for differences in application rate from field to field. DPR also adjusts the flux calibration factor for method of application. For example, application methods which include covering the field with a tarpaulin have a lower flux calibration factor than methods which do not employ tarpaulins. DPR does not adjust the flux calibration factor for effects of other parameters such as soil moisture and soil type due to lack of data.

Number of Acres

The total amount (pounds) of methyl bromide released to the air increases as the size of the treated area increases. DPR uses the ISCST model to calculate air concentrations in relation to the size of the treated area.

Weather Conditions

DPR has used conservative, but not worst-case weather conditions to calculate the size of buffer zones. DPR assumed the wind speed is three miles per hour, wind direction is constant for 24 hours, and atmospheric stability was class C for 24 hours.

DPR will revise the buffer zones using different weather assumptions. Buffer zones during nonwinter months (excluding November - February) will be established using regional weather data.

Buffer zones during winter months (November - February) will assume worst-case weather assumptions: wind speed is two miles per hour, wind direction is constant for 24 hours, and atmospheric stability is reflecting winter conditions.

Terrain

DPR assumes the worst-case terrain: flat and in a rural area.

Target Concentration

The target concentration is 0.21 parts per million as a 24-hour average.

To determine the size of the buffer zone, DPR inputs the flux calibration factor, number of acres, weather, and terrain into the ISCST model, and the model calculates the distance to the target concentration. Current buffer zones range from 30 to 2010 feet, depending on the flux calibration factor and number of acres.

References

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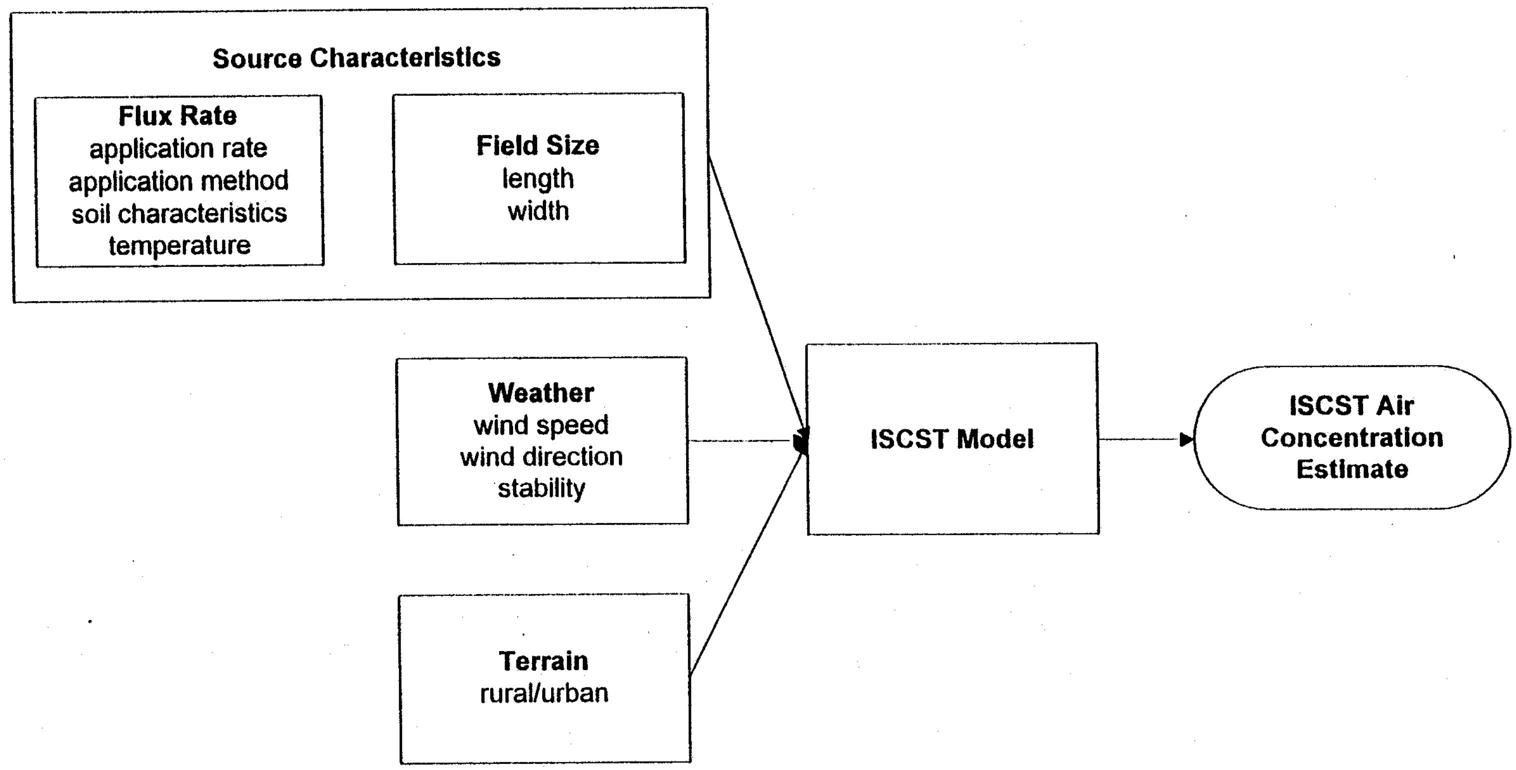
Figure 1. Industrial Source Complex-Short Term (ISCST) Computer Model



Relationship Between ISCST Estimate and Measured Air Concentration

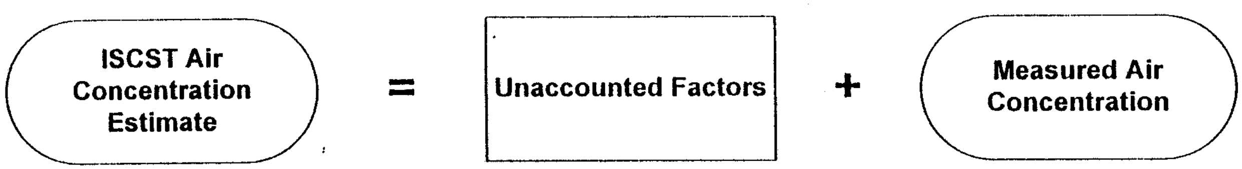


Figure 2. Back-Calculation Procedure Using ISCST Computer Model